



NBSIR 81-2219

Inventory Difference Calculations: Problems and Possibilities

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Final Report

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Nuclear Regulatory Commission
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U.S. DEPARTMENT OF COMMERCE, Malcolm Baldrige, *Secretary*
NATIONAL BUREAU OF STANDARDS, Ernest Ambler, *Director*

INVENTORY DIFFERENCE CALCULATIONS: PROBLEMS AND POSSIBILITIES

by J. A. Lechner

The origin, development, and termination of the "error study" task funded by the Nuclear Regulatory Commission at the National Bureau of Standards is presented in this report.

Other reports which grew (at least partially) out of this study are listed, and related to the intent of this study.

A general approach to the calculation of Inventory Difference (ID) and its Limit of Error (LEID) was devised and refined through visits to a selected fuel-fabrication facility. This approach is discussed, with emphasis on the importance of having measurements "under control" and on the possibility of automating the computations. The concepts of "measurement process" and "Measurement Assurance Program" are also discussed, and their importance shown. Possible problem areas, both those observed at the studied facility and others, are given, along with possible directions for resolution.

Finally, new approaches to the calculation of ID and LEID being developed elsewhere are described, and their relation to the approach being considered herein is elucidated.

1. Introduction and history.

In 1978 the National Bureau of Standards agreed to perform a task for the Nuclear Regulatory Commission. The purpose of this task was to investigate the nature of systematic errors. The task plan called for evaluating data currently available, to see if these data were sufficient to characterize the distribution of the systematic error components in material accounting. If the data were found to be sufficient, then they were to be used to perform the study and evaluate the characteristics of the systematic error components. If the data were found to be insufficient, then the measurement processes themselves were to be studied, and a determination was to be made of what would be necessary to properly evaluate the systematic errors. Several steps were envisioned. First, one licensee was to be chosen, acceptable to both NBS and NRC. The study was to be initiated with this licensee. At the conclusion of this phase, a report would be written, detailing the findings there and tentative generalizations to other licensees. The next step would be to verify these generalizations with smaller spot studies at other licensees.

Visits to the selected licensee began in December 1978. There were a total of six visits, of one or two days each, by one or two NBS personnel. In September 1979, after the sixth visit, it became apparent that there was a misunderstanding developing. The NRC inspectors were getting the impression that NBS had been hired by the licensee to correct some deficiencies noted in their material accounting system. At this point it was decided that there should be no communication between NBS and the licensee until this matter had been clarified. No further communication has occurred since that time. There have been several discussions between NBS and the sponsor at NRC, and attempts to initiate communication between NBS and the inspectors at NRC. This communication has not materialized. Funds have been

cut several times. Finally, the effort was terminated, with reports still to be written, and some of the necessary information still not obtained.

However, a considerable effort has gone into this study. Although the desired finished product has not been obtained, useful things have been learned at the licensee's facility. In addition, as a result of what was learned there, other studies have been carried forth, designed to improve the material accounting process. These are reported separately, and will be described only in general terms in this report. A general approach to material accounting, which allows for more systematic treatment of both the random and the systematic errors involved, was originated during the course of this study. It will be presented in this report. Its relationship to other approaches that have recently appeared will also be described. The concepts of measurement process and of measurement assurance program are also discussed, because they are vital to proper measurement control. Possible problem areas with this approach, both those observed at the studied facility and others, are given, along with possible directions for resolution.

2. Specific problems suggested by visits to the facility.

2.1 A fundamental problem, here as well as elsewhere in our experience, is the lack of a solid basis for the assessment of errors. This is due in part to the sophistication necessary to assess errors properly, and in part to insufficiency of data. This whole subject will be considered in Sections 3 and 4, because it is intimately connected to the idea of measurement as a process, and to the related concept of measurement assurance.

2.2 Another class of problems in calculating Limit of Error (LE) involves cancellation. The Inventory Difference (ID) is defined as $ID = (\text{Beginning Inventory}) + (\text{Receipts}) - (\text{Shipments}) - (\text{Ending Inventory})$, or $ID = BI + R - S - EI$. It is well-known that items appearing in both

Beginning Inventory and Ending Inventory cancel out of the equation for Inventory Difference, and thus contribute nothing to the LE. But items in BI and Shipments (S), or Receipts (R) and EI, or R and S, should also cancel. Furthermore, in some processes there is no chemical change to fuel material during the manufacturing process. Thus the accounting is by element, with percent U235 being the same for outgoing as for incoming material. (It may even be that percent U is the same, too.) In such a case, there can be no contribution to LE from the isotopic (and maybe also the chemistry) error, since the same value is used. If this sort of process represents a large portion of throughput, then the effect is significant. Of course, the fraction of material which gets recovered will be shipped with different chemistry and isotopic values, so that both input and output chemistry/isotopic errors apply to that fraction. The consideration here is similar to that applied in Reference [1], example 6.E, page 202ff where the isotopic error applies not to the entire throughput, but only to the ID. In our case, it applies not to the entire throughput but only to the ID and to all material which goes to Recovery.

2.3 It appears that oversimplified formulas may be in use for combining variances. In particular, at the facility studied, $(BI + R - S - EI)^2$ is calculated by material type, and multiplied by the appropriate (relative) systematic error variance. This is not correct, even if done separately for each value of the variance. It needs to be done separately for each separate value of the systematic error (even though the actual values are not known). For example, suppose that four made-up standards are used during the inventory period, and that the quantities $(BI+R-S-EI)$ measured with each standard are +50, -70, +100, -70, which total to +10. Assuming that the errors in

making up the standards are independent, the (relative) systematic error variance for these errors should be multiplied by $(50)^2 + (-70)^2 + (100)^2 + (-70)^2 = 22,300$, not by $10^2 = 100$, to obtain the contribution to LE from this error. (If the amounts were the same magnitudes but all positive, the correct multiplier is still 22,300, but the incorrect figure is 84,100. Thus the miscalculation could be in either direction.)

Finally, note that the total quantities measured with each standard should be used; this includes all types of material.

2.4 Problems also appear with the random error variance. For example, at the studied facility, the term $(BI_{type})^2 (\sigma^2_{rand type})/N$ appears. This is valid only when cancellation has been done properly, in the equation for ID, and when every item in the BI is of the same magnitude and subject to the same variance. If the magnitudes are different, but the (relative) error is the same, the formula will underestimate the total error. The effect is not serious for magnitudes in the same general size range. When the items differ from the mean item size by ± 10 percent at most, the resulting variance is underestimated by at most 1/2 percent. However, when the differences can be as large as ± 40 percent, the resulting variance is underestimated by up to 8 percent. Another problem arises, however, if the relative errors are not the same. For instance, if a scale has the same random error variance regardless of the weight, then the error variance is $n \cdot \sigma^2$ where n is the number of items weighed and σ is not a relative error but an absolute error (i.e., is not in percent but in grams). What one wants, in general, is simply the sum of the

absolute variances (i.e., in grams squared) for all the items weighed that period. (This is assuming that the ID involves simply the sum of the weights. For more complicated relationships, the usual propagation of error formulas can be applied.)

3. Measurement control and measurement assurance.

Measurements are the result of a process. Material is input to the process, and numbers are produced by the process. We may distinguish two modes of operation. If a given item is measured repetitively, the situation corresponds to a manufacturing process attempting to produce identical items. If on the other hand, a sequence of different items are measured, it is like a custom manufacturing process filling orders for different sizes of an item.

In the manufacturing process, the items produced will not be precisely the specified size(s), although the errors will be detected only if a sufficiently accurate inspection is performed. Likewise, measurements are not exact. However, there is a difference: when measuring unknowns, one has no specification against which to measure errors. For the manufacturing process, the quality is monitored by measuring the errors (actual value minus specification value) accurately for selected items. For a measurement process, one could imagine a more accurate measurement method (a "reference method" in a sense), used to measure the error made by the measurement process on selected items. Alternatively (and usually more conveniently) one could remeasure one or more specific items ("check standards") from time to time. The resulting measurement values can be treated just like the measurement errors in the manufacturing process, except that sometimes one does not know the "true value" for these check standards.

How are these values to be treated? In industry they are usually plotted on a "control chart", which embodies decision rules for flagging problems or potential problems in the manufacturing process. Similarly, measurements on a check standard can be used to flag problems or potential problems in the measurement process. Such use is called "measurement control" or "measurement assurance", short for measurement quality control or measurement quality assurance. Quality control has been the subject of many publications, from the early work of Shewhart [2], through the ASTM Manual of 1976 [3] and the Quality Control Handbook [4], to more recent work ([5], for example).

The starting point for measurement control is the attainment of a "state of statistical control" in the measurement process. Quoting Ref. 6, "... until a measurement operation ... has attained a state of statistical control it cannot be regarded in any logical sense as measuring anything at all." A sufficient condition for this state of control is that the errors in successive measurements are independent, identically distributed random variables. Generalization to situations more like much actual practice are discussed in Ref. [6], where the concept of "multistage statistical control" is expounded. This covers cases where there are certain components of error which remain fixed for periods of time but vary randomly between periods. Examples are periodic calibration and made-up standards.

To properly understand and use this approach, it is helpful to discuss the concepts of systematic error and random error. We start with the idea of a "limiting mean". This is a hypothetical value, the value that would be approached by the average as one takes more and more measurements under conditions specified as well as one knows how to specify: instrument,

operator, reference solutions, environment, etc. By definition, the difference between a given measurement and the limiting mean under the same conditions is a random error; and the difference between the limiting mean and the desired value (the "true value", possibly defined relative to a national standard) is the systematic error. Now this systematic error can be seen to depend on, among other things, the instrument, the operator, the temperature (and/or other environmental conditions), and perhaps even on the item itself. (This latter situation occurs, for example, when different barrels of scrap, containing the same amount of special nuclear material, will produce different (but stable) values on a drum counter because of geometry or other such factors. It also occurs when a calibration curve is used, because the inaccuracy in the curve is different for different amounts of material.) In this case, we have "item-dependent errors". A more complete discussion will be found in another of the reports growing out of this contract (Ref. [7]).

Assume the complication of item-dependency does not exist. One must still face up to the presence of systematic error which varies: over time, between operators, etc. One way to keep tabs on the process, i.e., to "assure" that both the systematic error and the random error are under control, is to use a "measurement assurance program". This usually involves frequent measurement of check standards, and occasional measurement of artifacts (whose true values are unknown to the participant) in exactly the same way that production measurements are made. The errors in measurements of the artifact are then an indication of systematic error in the measurement process. More detail on the measurement assurance program approach is to be found in References [8], [9], and [10]; the latter is concerned specifically with calibration.

In the absence of sufficient data of the type just mentioned, it is impossible to produce valid and "tight" uncertainty statements. More specifically, until the different sources of variation are properly assessed, the only valid estimates of uncertainty (and thus the estimates of LE) are larger than they need be.

4. Grassroots material accounting.

The inventory difference (ID) is a number, defined as (Beginning Inventory + Receipts - Shipments - Ending Inventory). It is calculated from other numbers, each one eventually expressible (in general) in terms of measurements of some sort:

$$ID = f(x_1, x_2, \dots, x_N)$$

where N may be several hundred (or even several thousand).

If the errors in all the x_i are independent, with mean zero and known variance σ_i^2 , then (to a first approximation, and assuming the function f is well behaved)

$$\text{var}(ID) = \sum_{i=1}^n \left(\frac{\partial f}{\partial x_i} \right)^2 \sigma_i^2 .$$

In this case, computation of the limit of error, LEID, is straightforward (although probably tedious) if σ_i 's and $\frac{\partial f}{\partial x_i}$'s are determinable. If the

errors are not independent, but do have mean zero, we need the covariance matrix of the set of x_i :

$$\text{var ID} = \sum_{i,j=1}^N \frac{\partial f}{\partial x_i} \frac{\partial f}{\partial x_j} \sigma_{ij} ,$$

where

$$\begin{aligned} \sigma_{ij} &\equiv \text{cov}(x_i, x_j), \text{ and} \\ \sigma_{ii} &\equiv \sigma_i^2 . \end{aligned}$$

4.1 Systematic errors.

But what happens when there are "systematic" errors? First, we need to be clear about the meaning of the term "systematic". It has long been applied to uncorrected biases, such as, the error due to an incorrect half life value. Hardly anyone will object to this use of the term. It has come to be applied to "components of variance", as for example when a new bottle of reagent is used each week, and the contribution due to the reagent variability is called a "short term systematic". Here a problem ensues: systematic errors have traditionally been thought of as (unknown) constants, but here they vary from day to day or week to week. For better or worse, this usage is by now thoroughly ingrained in the Safeguards community. Furthermore, the term "systematic error variance" is in common use, even in cases where the error is a constant. In this case, the term sometimes refers to the variance of the systematic error remaining after a (randomly determined) correction is applied, as in recalibration. Since the error remaining is the difference between the original (systematic) error and a random variable, it is also a random variable; its variance is identical to the variance of the (random) correction. Unfortunately, the term seems to imply that the systematic error itself is random, even when it is not. Furthermore, when the correction is deemed too small to apply, the "systematic error variance" is still recommended ([1]) to characterize the uncertainty due to that source of error. No clear justification exists for this approach. It is true that the variance of the correction estimate somehow measures how far from zero the true error could reasonably be expected to be, so that probabilistic limits on its extent can be derived. However, the error (whatever its true value is) is not necessarily a random error. The only truly appropriate way to handle such errors is to study them in enough detail and over enough time to characterize

their behavior. If a rule is used to determine when to "correct", then that rule must be considered also, so that the characteristics of the error that results (from applying or not applying corrections according to the rule) can be accurately modeled. One more point of possible confusion needs to be mentioned. Take, for example, the case of the reagent bottles. The bottle-to-bottle differences correspond to systematic errors. Suppose these differences were actually randomly distributed with variance σ^2 . This is then the "variance of the systematic error". Its value depends on the procedures which produced the bottles, and has nothing to do with the operations at the user's plant. Now suppose the value for a particular bottle is estimated (using a known standard) from a sequence of n independent determinations. If the variance of one determination is (say) σ_0^2 , then the variance of the average of n determinations will be σ_0^2/n . This quantity, which is also the variance of the estimate of the systematic error of a given bottle, is the "systematic error variance"; it is unrelated to σ^2 , and depends only on n and the accuracy of the n determinations. It is important to be careful which meaning is being used.

4.2 Independent case.

Now consider the situation where each of the x_i has, in addition to a random error, a defined pair of limits, say (Δ_i^-, Δ_i^+) , on its systematic error. If the systematic errors are unconnected, in the sense that knowing the actual systematic error for one of the x_i tells us nothing about the actual error for the others, the situation can be handled by splitting the x_i into two groups, based on the sign of $\frac{\partial f}{\partial x_i}$. We simply substitute $x_i + \Delta_i^+$ for x_i if $\frac{\partial f}{\partial x_i} > 0$, and $x_i + \Delta_i^-$ for x_i if $\frac{\partial f}{\partial x_i} < 0$, and calculate the new value of f ; and then repeat, using the other error limit for each x_i . This

procedure gives two values of f , whose differences from the original value are the limits of error due to the systematics; to these, one needs to add the appropriate multiple of the standard deviation of the ID.

4.3 Dependent case; removing correlation.

Finally, if the systematics are not "independent", the contribution from systematic error is more complicated. For example, $f(x)$ might include $x_{10} - x_{11}$, where in reality $x_{10} = Y + Z$ and $x_{11} = W + Z$, and the systematic error affects only Z . In terms of the x 's, the treatment above would inflate one of the x 's and deflate the other by the appropriate limits for systematic error. In terms of Y , Z , and W , however, it is obvious that the effect of systematic error on this part of ID is negligible: if systematic error inflates x_{10} , it must inflate x_{11} also, thus canceling out. This example shows the importance of expressing the measurements in terms of the basic error components. Incidentally, the same technique may also be applied when different measurement errors are correlated because they share a common component (for example, an error due to system setup, standards, operators, etc.). Note that the effect of the error is not removed; the resulting correlation is removed, thus simplifying the determination of valid LE's.

Another source of correlation is the use of calibration curves: each determination using the curve is a function of the (randomly-determined) parameters of the fitted curve, so that all the readings taken in an interval between recalibrations are correlated. In some cases, there is not even a closed-form expression for the inverse function, so it is not possible to express these values precisely in terms of the parameters. In fact, even for cases where the inverse curve is expressible in closed form, it does not

necessarily follow that the determinations even have finite variance. It is clear that calibration curves could cause complications, for which further work would be required. A recent report [11] on calibration goes into more detail.

The approach outlined above will avoid many pitfalls due to correlation, and will enable the explicit consideration of systematic error bounds. It is still necessary, of course, to obtain these bounds; for this, a statistically-designed study will usually be necessary.

4.4 Implementation.

The suggested approach, in simplest terms, is to express everything in the equation for ID in terms of the basic measurements which contribute errors, and then to collect terms so that the effect of each error can be clearly seen. Is this practical? Can one manage to accomplish this in a manufacturing facility, where the operating personnel who make measurements and do calculations are not statisticians? Perhaps so. Most facilities have already computerized their material accounting. The incorporation of a capability to perform the LE evaluation seems feasible. One approach will now be outlined, by example.

The computer system is assumed to have symbol manipulation capability. It will contain the actual numbers determined by various measuring systems, and distinct index numbers for each. It will also contain two other categories of information. One is a catalog of error information for the "basic" measurements in the system, which will contain the variance of the random component of error for that measurement and the limits (positive and negative) of systematic error for that measurement. The other is a list of symbolic expressions which express every other number in terms of the basic measurements. Now let us see by example how this would work.

Consider first an "assigned value" for an in-house mass standard, labeled (say) s17 in the computer file. The only significance of the number s17 is that there were 16 other values assigned to standards before this (not necessarily all for this standard). If there is no component of error common to this and to other measurements -e.g., this is the only standard calibrated against a given NBS standard, and the calibration was done in such a way that the assigned value has a random error independent of any other determinations and a systematic error dependent only on the NBS standard's value -then it qualifies as a "basic measurement". It would appear in the catalog (or rather, its index number would appear in the catalog) accompanied by values for the random-error variance and the appropriate systematic-error limits.

Now suppose this value were used, together with a comparative weighing sequence, to determine the weight of a product item. Further, let us suppose that the item is the 24th product item measured, and denote its measured value by p24. The operator would, of course, enter the measured value into the system, together with its index number, perhaps by entering the equation " $p_{24} = 41.235$ ". Now for this item, this number is all that is necessary to compute the ID. However, more is needed to compute a LE: the system needs to know the error characteristics of this number. So the operator also needs to input a symbolic expression to let the system know what to do with the number. He writes something like " $p_{24} = s_{17} + d_{36}$ ", which expresses the relationship between the determination p24 and the components which were used to obtain it, namely the assigned value s17 and a difference which was obtained in the comparative weighings. I have labeled this difference d36, as if there were 35 other differences before it. It is, of course, the difference

between the average product weight and the average weight of the standard in the sequence. Note that it qualifies as a "basic measurement" (under reasonable assumptions), because its systematic error is zero and its random error is independent of any other determination (as long as only one product item was present in the difference sequence). But the computer needs to know this. Therefore, the operator must also catalog the symbol d_{36} , by inserting into the system catalog this symbol, the random error variance, and the systematic error limits (zero in this case).

Proceeding in this fashion, one can keep a real-time check on the consistency of information entered. At the end of the accounting period, the computer can look at the equation for ID, determine the coefficients of the first-order expansion in terms of each variable around its measured value, and compute the contribution to LE due to errors in each variable in turn.

This report is not the place to present a finished system, because the contract did not fund such an effort. However, let's extend the example one step more. Suppose that not one but three different product items are weighed in one sequence with the in-house standard. Then the corresponding three differences are correlated, since they all contain the same term for the average weight of the standard. The treatment is only slightly more complicated, however. Instead of entering the differences as "basic measurements", the operator enters the three averages w_{36} , w_{37} , and w_{38} corresponding to the product cylinders, and the one average w_{39} corresponding to the standard, and the symbolic equations " $p_{24} = s_{17} + w_{36} - w_{39}$ ", " $p_{25} = s_{17} + w_{37} - w_{39}$ ", and " $p_{26} = s_{17} + w_{38} - w_{39}$ "; and he catalogs all four of these weights as basic variables, with the appropriate random error

variance and with no systematic error. (Actually, there is a systematic error in each weight, but by design this error is identical for each weight, and cancels out.) One might instead define variables corresponding to the systematic error, especially if one didn't know that these errors cancel out. The point is that it is not enough to use the same systematic error limits, since that approach would allow for systematic error in both terms independently instead of cancelling it out.

Finally, a few brief words about two other approaches in the literature. There are two somewhat similar programs which have been publicized recently: NUMSAS (see [12] and references cited there) and a program used by General Electric (Wilmington) [13]. In both, random and systematic errors are both taken to be characterized by a variance, with the mean assumed to be zero. The only errors considered are weighing, analytical, and sampling. Furthermore, the amount of SNM in each batch is assumed to be expressible as (bulk measurement) \times (uranium factor) \times (enrichment factor). The difference between the two is that the former models each transaction as a true value plus random error plus systematic error, and allows for common systematic errors by simply using the same error variable for all transactions which share that value of error; the latter stratifies the error sources, one error type at a time, by magnitude of the error variance. Thus it seems that the former allows for more detailed treatment of errors, while the latter shortens the computation by combining transactions. Neither allows for absolute limits the systematic errors; neither allows for unusual computations (like corrections based on residue analyses); and possibly, neither allows for the kind of partial cancellation that occurs when the same isotopic fraction is used for input as for (a large share of) output. However, these two programs are already operational.

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U.S. DEPT. OF COMM. BIBLIOGRAPHIC DATA SHEET (See instructions)	1. PUBLICATION OR REPORT NO. NBSIR 81-2219	2. Performing Organ. Report No.	3. Publication Date FEBRUARY 1981
4. TITLE AND SUBTITLE <p style="text-align: center;">INVENTORY DIFFERENCE CALCULATIONS: PROBLEMS AND POSSIBILITIES</p>			
5. AUTHOR(S) <p style="text-align: center;">J. A. Lechner</p>			
6. PERFORMING ORGANIZATION (If joint or other than NBS, see instructions) <p>NATIONAL BUREAU OF STANDARDS DEPARTMENT OF COMMERCE WASHINGTON, D.C. 20234</p>			7. Contract/Grant No. 8. Type of Report & Period Covered
9. SPONSORING ORGANIZATION NAME AND COMPLETE ADDRESS (Street, City, State, ZIP) <p>U.S. Nuclear Regulatory Commission Washington, DC 20555</p>			
10. SUPPLEMENTARY NOTES <input type="checkbox"/> Document describes a computer program; SF-185, FIPS Software Summary, is attached.			
11. ABSTRACT (A 200-word or less factual summary of most significant information. If document includes a significant bibliography or literature survey, mention it here) <p>The origin, development, and termination of the "error study" task funded by the Nuclear Regulatory Commission at the National Bureau of Standards is presented in this report.</p> <p>Other reports which grew (at least partially) out of this study are listed, and related to the intent of this study.</p> <p>A general approach to the calculation of Inventory Difference (ID) and its Limit of Error (LEID) was devised and refined through visits to a selected fuel-fabrication facility. This approach is discussed, with emphasis on the importance of having measurements "under control" and on the possibility of automating the computations. The concepts of "measurement process" and "Measurement Assurance Program" are also discussed, and their importance shown. Possible problem areas, both those observed at the studied facility and others, are given, along with possible directions for resolution.</p> <p>Finally, new approaches to the calculation of ID and LEID being developed elsewhere are described, and their relation to the approach being considered herein elucidated.</p>			
12. KEY WORDS (Six to twelve entries; alphabetical order; capitalize only proper names; and separate key words by semicolons) <p>inventory difference; limit of error; material accounting; Nuclear Regulatory Commission; systematic error.</p>			
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